2,3-Dibromothiophene 3140-93-0 | DTXSID80185324

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Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 89.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.34e-01

Confidence level: 7.54e-01

Nearest Neighbors from the Training Set

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Tetrachloroethylene Measured: 251 Predicted: 170

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Chloropicrin Measured: 61.7 Predicted: 61.7

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1,2-Dibromoethane Measured: 51.3 Predicted: 55.8

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1,2-Dibromo-3-chloropropane

Measured: 70.8 Predicted: 84.1

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1,1,2,2-Tetrachloroethane

Measured: 79.4 Predicted: 77.8